

APPENDIX - Enthalpy Data

Most of the thermochemical data have been taken from evaluations or reviews. In some cases, we have selected more recent experimental data, which appear to be reliable. The error limits are those given by the original author or reviewer.

Species	$\Delta_f H^\circ_{298}/\text{kJ mol}^{-1}$	$\Delta_f H^\circ_0/\text{kJ mol}^{-1}$	Reference
H	217.998 ± 0.006	216.03 ± 0.006	1
H ₂	0	0	1
O(³ P)	249.18 ± 0.10	246.79 ± 0.10	1
O(¹ D)	438.9	436.6	2
O ₂	0	0	1
O ₂ (¹ Δ)	94.3	94.3	2
O ₂ (¹ Σ)	156.9	156.9	2
O ₃	142.7	145.4	3
HO	37.20 ± 0.38	36.91 ± 0.38	65
HO ₂	14.6		4
H ₂ O	-241.826 ± 0.04	-238.92 ± 0.04	1
H ₂ O ₂	-136.31	-130.04	3
N	472.68 ± 0.40		1
N ₂	0	0	1
NH	352 ± 10		5
NH ₂	188.7 ± 1.3		4
NH ₃	-45.94 ± 0.35		1
NO	90.25	89.75	3
NO ₂	33.18	35.98	3
NO ₃	73.72 ± 1.4	78.95 ± 1.4	6
N ₂ O	82.05	85.500	3
N ₂ O ₄	9.1 ± 1.7	18.7 ± 1.7	7
N ₂ O ₅	11.3		6,7
HNO	112.95 ± 0.25	110.02 ± 0.25	8
HNO ₂	-79.5		3
HNO ₃	-135.06	-125.27	3
HO ₂ NO ₂	-52.7 ± 8		9
CH	596.4 ± 1.2		4
CH ₂ (³ B ₁)	390.4 ± 4		4
CH ₂ (¹ A ₁)	428.3 ± 4		4
CH ₃	146.4 ± 0.4		4
CH ₄	-74.81	-66.818	3
CN	441.4 ± 4.6		4
HCN	135 ± 8		7
HCO	43.1		10,11
CH ₂ O	-108.6	-104.7	2
CH ₃ O	17.2 ± 3.8		4
CH ₂ OH	-17.8 ± 1.3	-11.5 ± 1.3	12
CH ₃ OH	-201.6 ± 0.2		13
CO	-110.53 ± 0.17		1
NCO	127.0		4
HOCO	-217 ± 10	-205 ± 10	4,14
HCOOH	-378.8 ± 0.5	-371.6	13
CH ₃ O ₂	9.0 ± 5.1		4
CH ₃ OOH	-131		7
HOCH ₂ O ₂	-162.1 ± 2.1		15

APPENDIX I (continued)

Species	$\Delta_f H^\circ_{298}/\text{kJ mol}^{-1}$	$\Delta_f H^\circ_0/\text{kJ mol}^{-1}$	Reference
CH ₃ ONO	-65.3		16
CH ₃ ONO ₂	-119.7		16
CH ₃ O ₂ NO ₂	-44		17
CO ₂	-393.51 ± 0.13		1
C ₂ H	566.1 ± 2.9		4
C ₂ H ₂	228.0 ± 1.0		13
C ₂ H ₃	300.0 ± 3.4		4
C ₂ H ₄	52.2 ± 1.2		13
C ₂ H ₅	120.9 ± 1.6		4
C ₂ H ₆	-84.0 ± 0.2		13
CH ₂ CN	243.1 ± 11.3		4
CH ₃ CN	74.0		18
CH ₂ CO	-47.7 ± 1.6		19
CH ₃ CO	-10.0 ± 1.2		4
CH ₂ CHO	10.5 ± 9.2		4
CH=CHOH		120 ± 10	20
CH ₃ CHO	-165.8 ± 0.4		13,21
C ₂ H ₅ O	-15.5 ± 3.4		4
C ₂ H ₄ OH		-23 ± 6	20
CH ₃ CHOH	-51.6		4
C ₂ H ₅ OH	-234.8 ± 0.2		13,21
(CHO) ₂	-211.9 ± 0.8		13,21
CH ₃ CO ₂	-207.5 ± 4		4
CH ₃ CO ₂ H	-432.14 ± 0.4		13,21
C ₂ H ₅ O ₂	-27.4 ± 9.9		4
CH ₃ OOCH ₃	-125.7 ± 1.3		13,21
CH ₃ C(O)O ₂	-172 ± 20		4
C ₂ H ₅ ONO	-103.8		13,21
C ₂ H ₅ ONO ₂	-154.1 ± 1.0		13,21
C ₂ H ₅ O ₂ NO ₂	-63.2		22
CH ₃ C(O)O ₂ NO ₂	-258 ± 22		23
CH ₂ =CHCH ₂	170.7 ± 8.8		4
C ₃ H ₆	20.2 ± 0.4		13,21
n-C ₃ H ₇	100.8 ± 2.1		4
i-C ₃ H ₇	86.6 ± 2.0		4
C ₃ H ₈	-104.5 ± 0.3		13,21
C ₂ H ₅ CO	-32.3 ± 4.2		24,25
CH ₃ COCH ₂	-23.9 ± 10.9		4
C ₂ H ₅ CHO	-187.4 ± 1.5		13,21
CH ₃ COCH ₃	-217.2 ± 0.4		13,21
C ₃ H ₆ OH	-74		16
n-C ₃ H ₇ O	-41.4		4
i-C ₃ H ₇ O	-52.3		4
i-C ₃ H ₇ OH	-272.5 ± 0.4		13,21
CH ₃ COCHO	-271.1 ± 4.7		13,21
C ₃ H ₅ O ₂	87.9 ± 5.5		4
i-C ₃ H ₇ O ₂	-68.8 ± 11.3		4
n-C ₃ H ₇ ONO ₂	-174.1 ± 1.3		13,21
i-C ₃ H ₇ ONO ₂	-190.8 ± 1.7		13,21
n-C ₄ H ₉	80.9 ± 2.2		4
s-C ₄ H ₉	66.7 ± 2.1		4

APPENDIX I (continued)

Species	$\Delta_f H^\circ_{298}/\text{kJ mol}^{-1}$	$\Delta_f H^\circ_0/\text{kJ mol}^{-1}$	Reference
n-C ₄ H ₁₀	-125.7 ± 0.4		13
n-C ₃ H ₇ CHO	-204.8 ± 1.5		13
CH ₃ COC ₂ H ₅	-238.5 ± 0.5		13
n-C ₄ H ₉ O	-62.8		4
s-C ₄ H ₉ O	-69.5 ± 3.3		4
S	277.17 ± 0.15		1
HS	143.01 ± 2.85	142.55 ± 3.01	26
H ₂ S	-20.6 ± 0.5		1
HSO	-4		4
SO	5.0 ± 1.3	5.0 ± 1.3	7
HSO ₂	-222		4
SO ₂	-296.81 ± 0.20		1
HOSO ₂	-385		4
SO ₃	-395.72	-389.99	3
HSNO	94		27
CH ₃ S	124.60 ± 1.84		26
CH ₃ SH	-22.9 ± 0.6		28
CH ₃ SCH ₂	136.8 ± 5.9		4
CH ₃ SCH ₃	-37.24	-21.058	3
CS	278.5 ± 3.8		4
CH ₃ SO	-67 ± 10		29
CH ₃ SOO	75.7 ± 4.2	87.9 ± 4.6	30
OCS	-142.09	-142.218	3
S ₂	128.60		1
CH ₃ SS	68.6 ± 8		4
CH ₃ SSCH ₃	-24.3		31
CS ₂	117.36	116.57	3
HOCS ₂	110.5 ± 4.6		32
F	79.38 ± 0.30		1
HF	-273.30 ± 0.70		1
HO ₂ F	-98.3 ± 4.2	-95.4 ± 4.2	7
FO	109 ± 10	108 ± 10	7
FO ₂	25.4 ± 2	27.2 ± 2	7
FONO	67		33
FNO ₂	-108.8		17
FONO ₂	10	18	7
CH ₂ F	-31.8 ± 8.4		4
CH ₃ F	-232.6		34
CH ₃ CH ₂ F	-263 ± 2		35
HCOF		-392.5 ± 6.3	36
FCO	-152.1 ± 12	-172 ± 63	4
F ₂	0	0	1
CHF ₂	-238.9 ± 4		4
CH ₂ F ₂	-453 ± 8		35
CH ₃ CHF ₂	-501 ± 6		35
CF ₂	-184.1 ± 8.4		4
COF ₂	-634.7	-631.57	3
CHF ₃	-697.6		35
CF ₃	-466.1 ± 3.8		4
CH ₂ CF ₃	-517.1 ± 5.0		4

APPENDIX I (continued)

Species	$\Delta_f H^\circ_{298}/\text{kJ mol}^{-1}$	$\Delta_f H^\circ_0/\text{kJ mol}^{-1}$	Reference
CH ₃ CF ₃	-748.7 ± 3.2		37
CH ₂ FCHF ₂	-691 ± 10		37
CF ₃ O	-655.6 ± 6.3		38
CF ₃ OH	-923.4 ± 13.4		39
CF ₃ OF	-785		35
CF ₃ O ₂	-614.0 ± 15.4		15
CF ₃ CO ₂ H	-1031		28
CF ₃ O ₂ NO ₂	-686		22
CF ₄	-933	-927	40
Cl	121.301 ± 0.008		1
HCl	-92.31 ± 0.10		1
HOCl	-78	-75	2,41
ClO	101.63 ± 0.1		7
ClOO	97.457	99.128	42
OCIO	94.6 ± 1.3		43
sym-ClO ₃	217.2 ± 21		44
ClNO	51.7	53.6	7
ClNO ₂	12.5	17.95	3
ClONO	56		17
ClONO ₂	22.9 ± 2.2		45
CH ₂ Cl	117.3 ± 3.1		4
CH ₂ ClO ₂	-5.1 ± 13.6		4
CH ₃ Cl	-81.96 ± 0.67	-74.04 ± 0.67	40
CHF ₂ Cl	-483.7 ± 5.9		46
CH ₃ CHFCI	-313.4 ± 2.6		37
CH ₃ CF ₂ Cl	-536.2 ± 5.2		37
ClCO	-21.8 ± 2.5	-23.4 ± 2.9	47
COFCI	-427	-423	7
CFCl	31.0 ± 13.4		4
CF ₂ Cl	-279.1 ± 8.3		4
CF ₂ ClO ₂	-406.5 ± 14.6		15
CF ₂ ClO ₂ NO ₂	-480		48
CF ₃ Cl	-707.9 ± 3.8	-702.8 ± 3.8	46
Cl ₂	0	0	1
Cl ₂ O	77.2 ± 3.4		49
Cl ₂ O ₂	127.6 ± 2.9		43
Cl ₂ O ₃	153		50
CCl ₂	230.1 ± 8.4		4
CHCl ₂	89.0 ± 3.0		4
CHCl ₂ O ₂	-19.2 ± 11.2		4
CH ₂ Cl ₂	-95.4 ± 0.8	-88.5 ± 0.8	40
CHFCI ₂	-284.9 ± 8.8		46
COCl ₂	-220.1	-218.4	7
CFCl ₂	-89.1 ± 10.0		4
CFCl ₂ O ₂	-213.7		4
CFCl ₂ O ₂ NO ₂	-287.4		48
CF ₂ Cl ₂	-493.3 ± 2.5	-489.1 ± 2.5	46
CH ₂ ClCF ₂ Cl	-543 ± 10		35
CF ₃ CHCl ₂	-740 ± 10		35
CF ₂ ClCHFCI	-724 ± 10		35

APPENDIX I (continued)

Species	$\Delta_f H^\circ_{298}/\text{kJ mol}^{-1}$	$\Delta_f H^\circ_0/\text{kJ mol}^{-1}$	Reference
CF ₂ ClCF ₂ Cl	-925.5 ± 4.3		37
CCl ₃	71.1 ± 2.5	69.9 ± 2.5	51
CCl ₃ O ₂	-20.9 ± 8.9		4
CCl ₃ O ₂ NO ₂	-83.7		48
CHCl ₃	-103.3 ± 1.3		7
C ₂ HCl ₃	-7.78	-4.318	3
CH ₃ CCl ₃	-144.6 ± 0.8		37
CFCl ₃	-284.9 ± 1.7	-281.1	46
CF ₂ ClCFCl ₂	-726.8 ± 2.8		37
CCl ₄	-95.8 ± 0.6	-93.6 ± 0.6	40
C ₂ Cl ₄	-12.4	-11.9	7
C ₂ Cl ₅	33.5 ± 5.4	33.9 ± 6.3	52
Br	111.87 ± 0.12		1
HBr	-36.29 ± 0.16		1
HOBr	≥ -56		53
BrO	119.7 ± 5.9		54
OBBrO	163.9 ± 4.4	172.9 ± 4.4	66
BrOO	108 ± 40	116 ± 40	7
BrNO	82.17	91.46	3
BrONO ₂	42.3 ± 8		55
CH ₂ Br	169.0 ± 4.2		4
CH ₃ Br	-38.1 ± 1.3		13
CH ₂ ClBr	-20 ± 7		56
CF ₃ Br	-650		35
CF ₂ ClBr	-438 ± 8		35
BrCl	14.6 ± 1.3	22.1 ± 1.3	7
Br ₂ (g)	30.91		1
Br ₂ O	107.1 ± 3.5		57
Br ₂ O ₂	181 ± 12		58
CHBr ₂	188.3 ± 9.2		4
CH ₂ Br ₂	-11.1 ± 5.0		59
CF ₂ Br ₂	-379 ± 8		35
CF ₂ BrCF ₂ Br	-789.9		37
CHBr ₃	23.8 ± 4.5		59
I	106.76 ± 0.04		1
HI	26.50		1
HOI	-69.6 ± 5.4	-64.9	60,61
IO	115.9 ± 5.0		62
INO	121.3 ± 4.2	124.3 ± 4.2	63
INO ₂	60.2 ± 4.2	66.5 ± 4.2	63
CH ₂ I	230.1 ± 6.7		4
CH ₃ I	14.2 ± 0.9		13
CF ₃ I	-589.1 ± 3.3		7
CH ₂ ClI	~7.1		34
CH ₂ BrI	~61.9		34
ICl	17.5 ± 0.1	19.1 ± 0.1	7
IBr	40.9 ± 0.1	49.8 ± 0.1	7
I ₂ (g)	62.42 ± 0.08		1
CH ₂ I ₂	118 ± 4		64

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